A Recent Perspective on Predictive Computational Science: Educational Needs and Opportunities

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Sandia is a multiprogram laboratory operated by Sandia Corporation, a Lockheed Martin Company, for the United States Department of Energy's National Nuclear Security Administration under contract DE-AC04-94AL85000.

Outline

- Overview of driving forces behind computational science at Sandia National Labs
- Predictive computational science
  - Verification
  - Uncertainty Quantification
  - Validation
- Automatic differentiation as a vehicle for transformation to predictive science
- Educational needs and opportunities

Sandia National Laboratories

Brief Overview of Sandia National Labs

- Founded in 1945 during the Manhattan Project
  - Primary mission was to design, produce and test all non-nuclear components of nuclear weapons
    - Security systems
    - Arming and fuzing systems
    - Safety systems
    - Instrumentation
    - Parachute systems and aerodynamic design
- Labs are located in Albuquerque, NM and Livermore, CA
  - Employ approx. 8,500 people (18% PhD)
- Managed by Sandia Corporation, a subsidiary of Lockheed Martin Corporation, for the National Nuclear Security Administration (NNSA, part of DOE)
  - Lab employees are DOE contractors

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Sandia Has Many Diversified Missions

- Nuclear Weapon Stockpile Stewardship
  - Ensure the stockpile is safe, secure, reliable, and can support the United States' deterrence policy
- Nonproliferation and Assessments
  - Reduce the proliferation of weapons of mass destruction, the threat of nuclear accidents, and the potential for damage to the environment
- Military Technologies and Applications
  - Address new threats to national security
- Energy and Infrastructure Assurance
  - Enhance the surety of energy and other critical infrastructures
- Homeland Security
  - Help protect our nation against terrorism

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NW Stockpile Stewardship is Sandia's Primary Mission

- Weapons are currently no longer produced
- Sandia's primary mission is to ensure the existing stockpile is
  - Safe
    - Ensure weapons don't detonate after an accident (plane crash, fire, etc…)
  - Secure
    - Ensure weapons cannot be detonated without authorization
  - Reliable
    - Ensure there is no degradation of performance over time
- Sandia does yearly testing to assess and certify the stockpile
  - Destructively and non-destructively test individual components and systems of weapons in the stockpile
  - By treaty, there are no underground nuclear test detonations

Science-Based Stockpile Stewardship Leads to Predictive Computational Science

- Problems with a solely testing-based approach
  - Eventually you run out of weapons to test
  - Without underground testing, you can't test the complete system
  - Not predictive
- Science-based stockpile stewardship
  - Develop comprehensive scientific models to assess safety, security, reliability of weapons
    - Understand how materials age
    - Effects of abnormal environments (heat, radiation, etc…)
    - Effects of imperfections, impurities, etc…
  - Using
    - Testing
    - Experimentation
    - Modeling
    - Computation

Predictive Computational Science

ASC™

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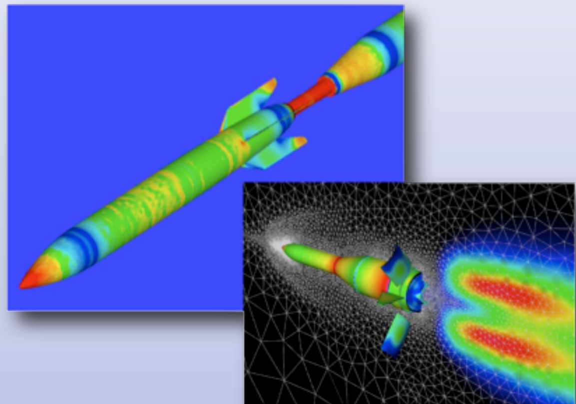
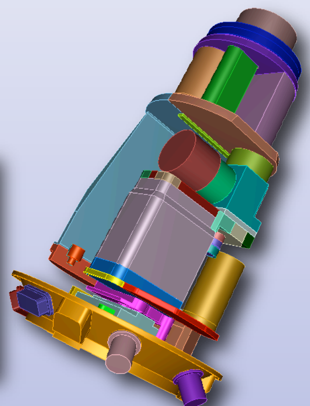
A Sampling of Areas of Interest for Predictive Computational Science

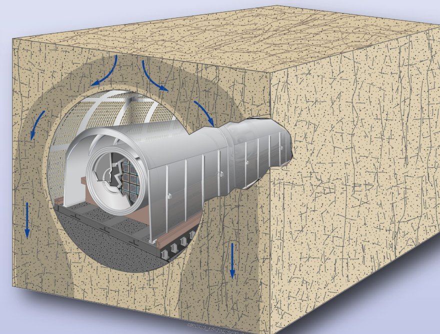
Aerodynamics



Structures

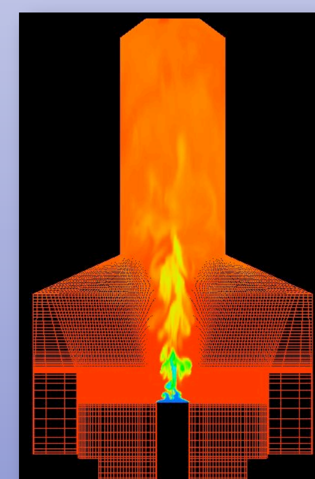


Waste Repositories

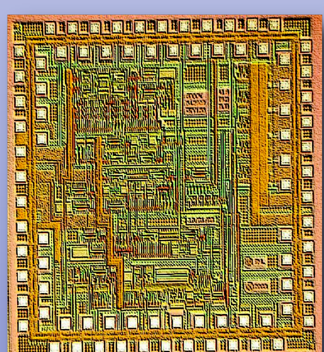


MEMS

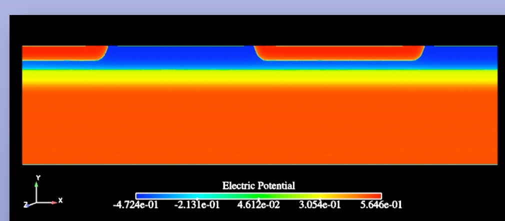
Combustion



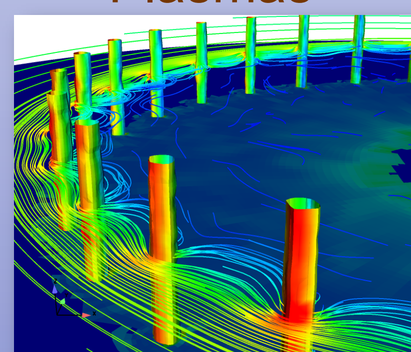
Circuits



Semiconductors

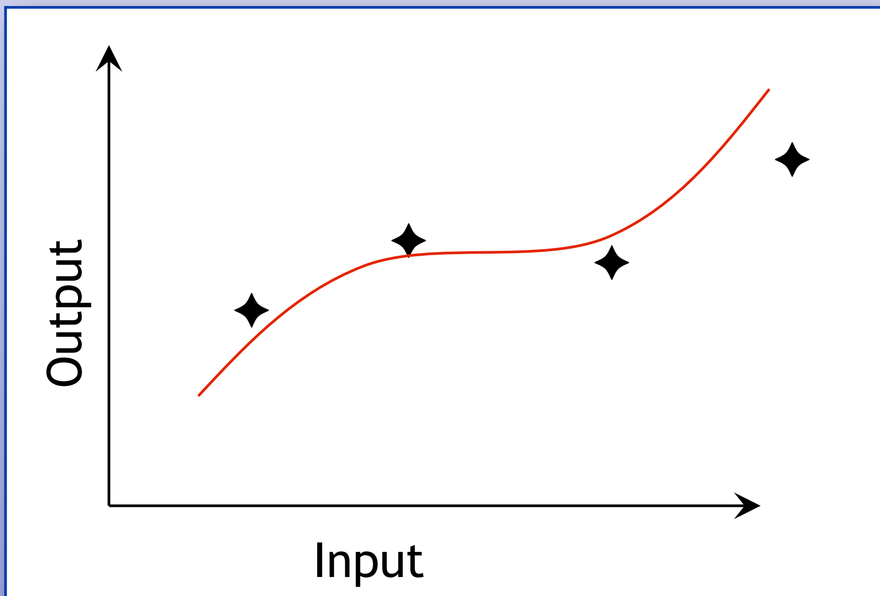


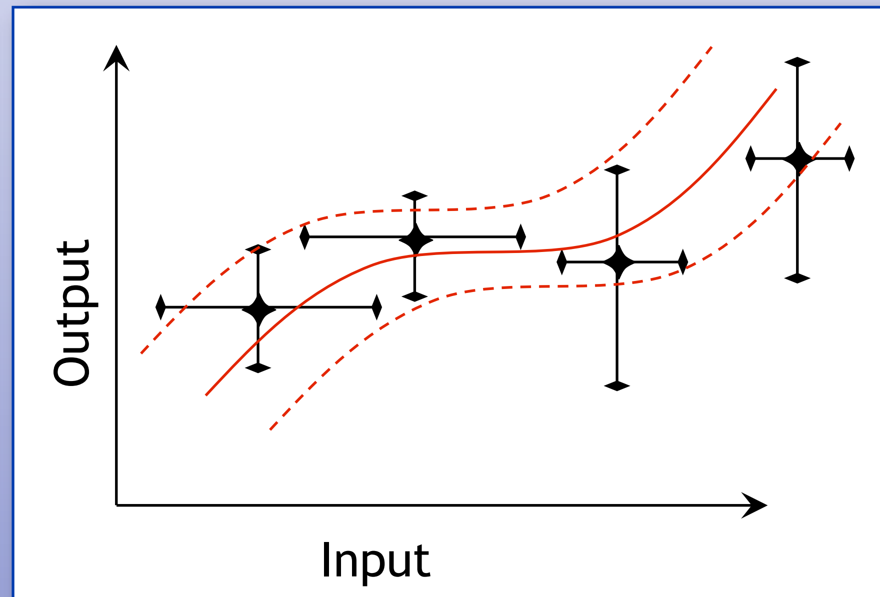
Plasmas



What Does "Predictive Computational Science" Mean?

- A scientifically credible and justifiable statement that a computation is capable of adequately capturing a physical/natural process.
  - Expert opinion is not sufficient
  - This was not readily apparent to the original ASC program





  - Verification, Uncertainty Quantification and Validation

Verification

- The process of determining that a model implementation accurately represents the developer's conceptual description of the model and the solution to the model.
  – "Are the equations solved correctly?"
- Code verification:
  – Finding and removing source code mistakes (bugs)
  – Improving software using software quality assurance practices (SQA)
- Solution verification:
  – Estimating numerical solution error
    - Grid refinement studies
    - Method of manufactured solutions
    - A posteriori error estimation
  – Assuring accuracy of simulation input and output data

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Uncertainty Quantification

- Process for determining how incomplete knowledge or variability of simulation inputs impact simulation results
  - Characterization of input uncertainties
  - Propagation of uncertainties through simulation to outputs
- Epistemic uncertainty -- “Lack of knowledge”
  - Set representations
  - Interval arithmetic
  - Possibility/Evidence theory
- Aleatory uncertainty -- “Intrinsic variability”
  - Probabilistic representations
  - Monte Carlo sampling and its many variants (LHS, importance,…)
  - Stochastic collocation
  - Polynomial chaos and other “spectral” projections

Validation

- The process of determining the degree to which a model is an accurate representation of the real world from the perspective of the intended uses of the model.
  - "Are we solving the correct equations?"
- Comparison of computational predictions to experimental observations
  - Quantitative assessment of experimental errors
  - Quantitative assessment of total computational error (numerical error + uncertainty)
  - Identification of a metric indicating whether simulation and experiment "agree"

So What's the Problem?

- V&V + UQ define a formal process for justifying predictive capability
  - Doesn't say how to do it
  - Doesn't say what to do when it doesn't work
    - May not understand the physics
    - May not be able to simulate at necessary level of fidelity
    - May not be able to measure all uncertainties/errors
    - May not have enough data
- Clearly significant challenges must be overcome
  - Accurate and efficient error estimation
  - Efficient uncertainty propagation for
    - strongly nonlinear problems
    - problems with discontinuities over parameter domain
  - Design of validation metrics

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Transformation to Predictive Science

- Computers, Computation, Information, and Mathematics Center (CCIM) is trying to lead transformation to predictive science at Sandia
  - Algorithms research
  - Incorporating state-of-the-art algorithms in production physics simulation codes

- Obtaining accurate derivatives efficiently has been one of the most significant hurdles
  - Focusing on Automatic Differentiation as a general technique for getting derivatives out of application codes

What Do Derivatives Have To Do With Predictive Science

- Verification
  - Adjoint-based error estimation
  - Sensitivity analysis to identify dominant physics
- Uncertainty quantification
  - Taylor expansions for uncertainty propagation
  - Identifying bifurcations for failure modes
  - Inverse problems for deducing uncertainty representations based on data
  - Optimization under uncertainty
- Validation
  - Adjoint-based parameter estimation and model calibration

Automatic Differentiation is an Enabling Technology for Predictive Science

- Analytic derivatives improve robustness and efficiency
  - Very hard to make finite differences accurate
- Infeasible to expect application developers to code analytic derivatives
  - Time consuming, error prone, and difficult to verify
  - Thousands of possible parameters in a large code
  - Developers must understand what derivatives are needed
- Not having analytic derivatives has been significant hurdle to predictive science research
- Automatic differentiation solves these problems

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What is Automatic Differentiation (AD)?

- Technique to compute analytic derivatives without hand-coding the derivative computation
- How does it work -- freshman calculus
  - Computations are composition of simple operations (+, *, sin(), etc…) with known derivatives
  - Derivatives computed line-by-line, combined via chain rule
- Derivatives accurate as original computation
  - No finite-difference truncation errors
- Provides analytic derivatives without the time and effort of hand-coding them

$$y = \sin(e^x + x\log x), \quad x = 2$$

		x	$\frac{d}{dx}$
$x \leftarrow 2$	$\frac{dx}{dx} \leftarrow 1$	2.000	1.000
$t \leftarrow e^x$	$\frac{dt}{dx} \leftarrow t\frac{dx}{dx}$	7.389	7.389
$u \leftarrow \log x$	$\frac{du}{dx} \leftarrow \frac{1}{x}\frac{dx}{dx}$	0.301	0.500
$v \leftarrow xu$	$\frac{dv}{dx} \leftarrow u\frac{dx}{dx} + x\frac{du}{dx}$	0.602	1.301
$w \leftarrow t + v$	$\frac{dw}{dx} \leftarrow \frac{dt}{dx} + \frac{dv}{dx}$	7.991	8.690
$y \leftarrow \sin w$	$\frac{dy}{dx} \leftarrow \cos(w)\frac{dw}{dx}$	0.991	-1.188

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How is AD Implemented?

- Source transformation
  - Preprocessor implements AD
  - Very efficient derivative code
  - Works well for FORTRAN, some C
  - Extremely difficult for C++
  - OpenAD, ADIFOR, ADIC (Argonne National Lab & Rice University)
- Operator overloading
  - All intrinsic operations/elementary operations overloaded for AD data types
  - Change data types in code from floats/doubles to AD types
    - C++ templates greatly help
  - Easy to incorporate into C++ codes
  - Slower than source transformation due to function call overhead
  - ADOL-C (TU-Desden), Sacado (Sandia), MAD (matlab)

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How is AD Used In Computational Science?

- Most AD uses have focused on black-box application
  - Trying to live up to the name "automatic"
- AD is better used selectively as a software engineering tool
  - Only use AD for the hard nonlinear parts
  - Don't use AD on solvers

Spatially discretized PDE:

$$f(\dot{u}, u, p, t) = 0$$

Temporal discretization (Backward Euler):

$$f\left(\frac{u_n - u_{n-1}}{\Delta t}, u_n, p, t_n\right) = 0$$

Forward sensitivity problem:

$$\frac{\partial f}{\partial \dot{u}}\left(\frac{\partial \dot{u}}{\partial p}\right) + \frac{\partial f}{\partial u}\left(\frac{\partial u}{\partial p}\right) + \frac{\partial f}{\partial p} = 0$$

$$\frac{1}{\Delta t}\frac{\partial f}{\partial \dot{u}}\left(\frac{\partial u_n}{\partial p} - \frac{\partial u_{n-1}}{\partial p}\right) + \frac{\partial f}{\partial u}\left(\frac{\partial u_n}{\partial p}\right) + \frac{\partial f}{\partial p} = 0$$

Element decomposition:

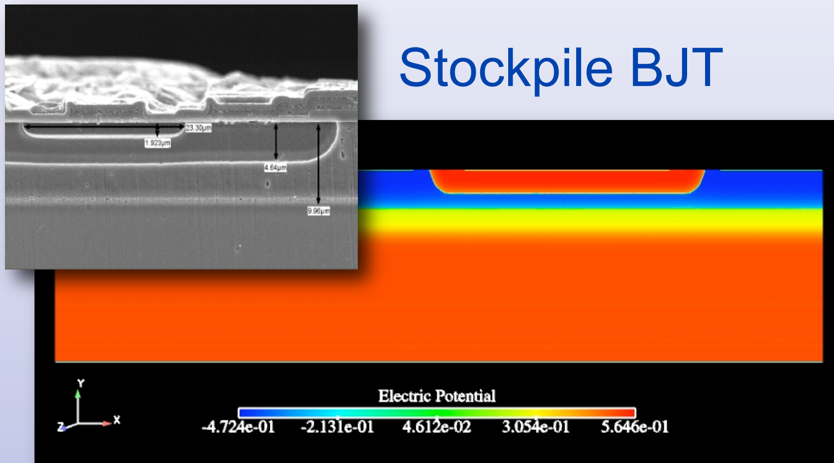
$$f(\dot{u}, u, p, t) = \sum_{i=1}^{N} Q_i^T e_{k_i}(P_i \dot{u}, P_i u, p, t)$$

$$\frac{1}{\Delta t}\frac{\partial f}{\partial \dot{u}} + \frac{\partial f}{\partial u} = \sum_{i=1}^{N} Q_i^T \left(\frac{1}{\Delta t}\frac{\partial e_{k_i}}{\partial \dot{u}_i} + \frac{\partial e_{k_i}}{\partial u_i}\right) P_i$$

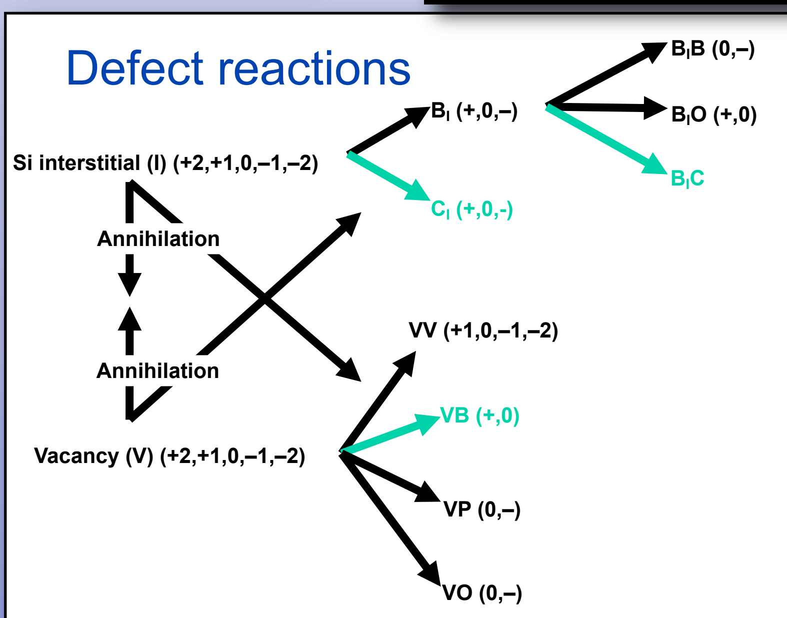
QASPR

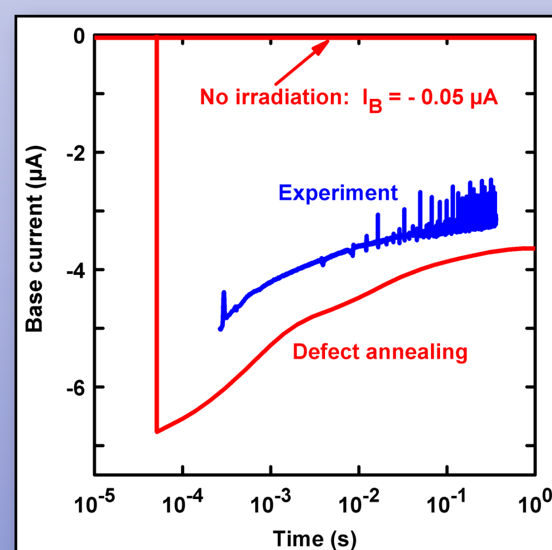
Qualification of electronic devices in hostile environments

Stockpile BJT



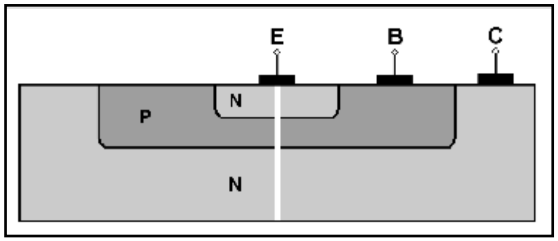
PDE semiconductor device simulation



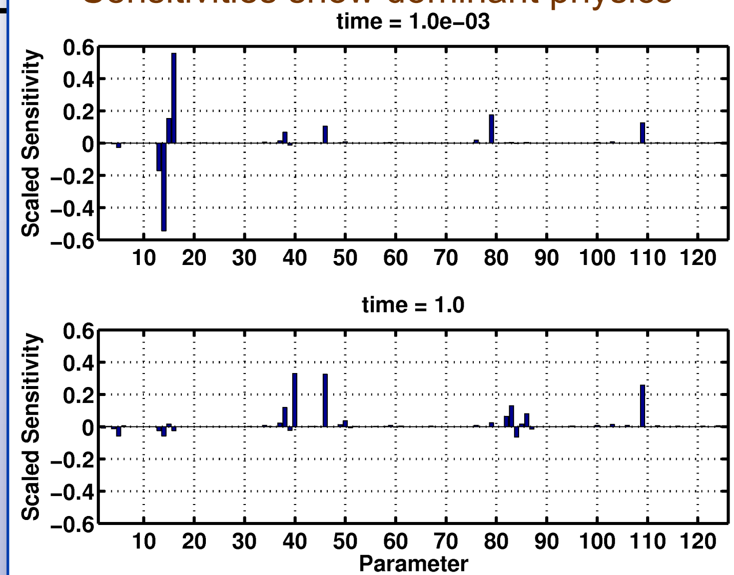


Transient Sensitivity Analysis of a Bipolar Junction Transistor Under Radiation

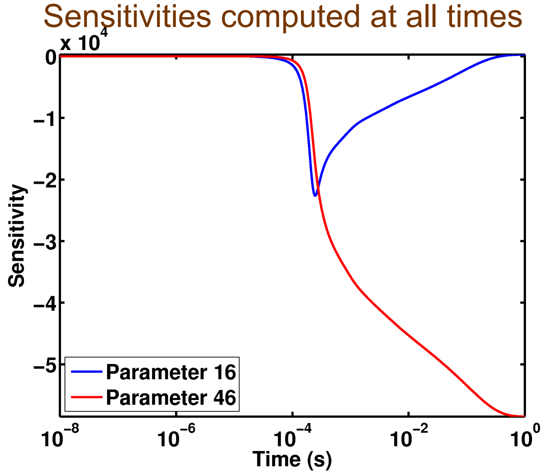
- Bipolar Junction Transistor
- Pseudo 1D strip (9x0.1 micron)
- Full defect physics
- 126 parameters



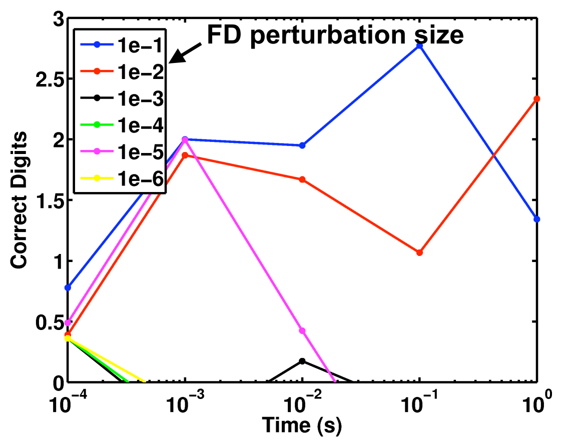
Sensitivities show dominant physics



Sensitivities computed at all times



1st-order Finite Difference Accuracy



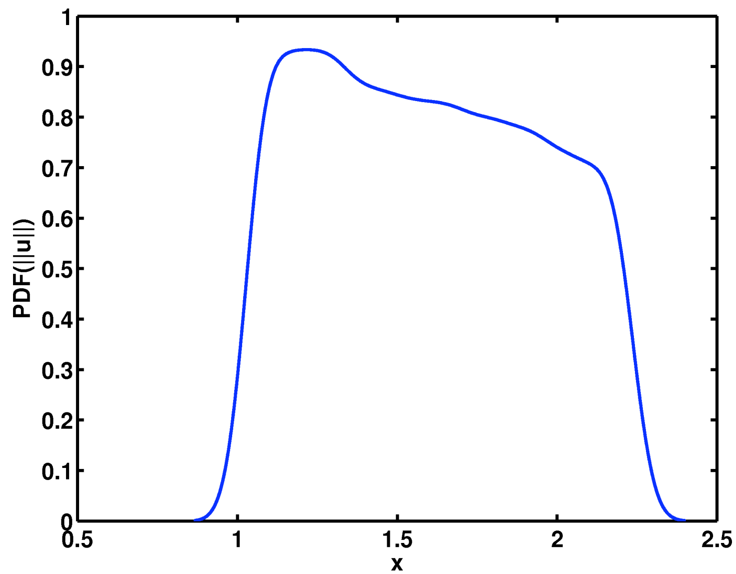
Comparison to FD:

- ✓ Sensitivities at all time points
- ✓ More accurate
- ✓ More robust
- ✓ 14x faster!

Moving Beyond Forward Sensitivities

- We are building on this technology for
  - Adjoint sensitivities
  - Second derivatives (SQP optimization)
  - Taylor polynomials (Time integration, UQ)
- We are also investigating AD-like ideas for calculations beyond derivatives
  - Polynomial chaos expansions for UQ

$$\nabla^2 u + \alpha e^u = 0, \quad \alpha \in [0.5, 1.5]$$



Educational Needs and Opportunities

- Must change culture for predictive computational science to be successful
  - Single-point forward simulations are not sufficient
- By emphasizing these ideas in undergraduate/graduate education, we can get there
- AD in particular is proving to be an important piece of the solution
- Significant progress could be made by exposing AD early in undergraduate education/research
  - Prerequisites are basic calculus and programming skills

AD Takes Two Basic Forms

$$x \in \mathrm{R}^n,\ f : \mathrm{R}^n \rightarrow \mathrm{R}^m,\ y = f(x) \in \mathrm{R}^m$$

- Forward Mode:
  - Propagate derivatives of intermediate variables w.r.t. independent variables *forward*

$$c = \varphi(a,b) \implies \frac{\partial c}{\partial x_i} = \frac{\partial \varphi}{\partial a}\frac{\partial a}{\partial x_i} + \frac{\partial \varphi}{\partial b}\frac{\partial b}{\partial x_i}$$

  - Change of variables

$$x = Vz,\quad V \in \mathrm{R}^{n\times p} \implies \frac{\partial y}{\partial z} = \frac{\partial f}{\partial x}V$$

  - Complexity

$$\text{ops}\left(f,\ \frac{\partial f}{\partial x}V\right) \approx (1 + 1.5p)\text{ops}(f)$$

- Reverse Mode:
  - Propagate derivatives of dependent variables w.r.t. intermediate variables *backwards*

$$c = \varphi(a,b) \implies \frac{\partial y_j}{\partial a} = \frac{\partial y_j}{\partial c}\frac{\partial \varphi}{\partial a},\quad \frac{\partial y_j}{\partial b} = \frac{\partial y_j}{\partial c}\frac{\partial \varphi}{\partial b}$$

  - Change of variables

$$z = W^T y,\quad W \in \mathrm{R}^{m\times q} \implies \frac{\partial z}{\partial x} = W^T\frac{\partial f}{\partial x}$$

  - Complexity

$$\text{ops}\left(f,\ W^T\frac{\partial f}{\partial x}\right) \approx (1.5 + 2.5q)\text{ops}(f)$$

Charon Drift-Diffusion Formulation with Defects

Current Conservation for e- and h+

$$\frac{\partial n}{\partial t} - \nabla \cdot J_n = -R_n(\psi, n, p, Y_1, \ldots, Y_N), \quad J_n = -n\mu_n \nabla\psi + D_n \nabla n$$

$$\frac{\partial p}{\partial t} + \nabla \cdot J_p = -R_p(\psi, n, p, Y_1, \ldots, Y_N), \quad J_p = -p\mu_p \nabla\psi - D_p \nabla p$$

Defect Continuity

$$\frac{\partial Y_i}{\partial t} + \nabla \cdot J_{Y_i} = -R_{Y_i}(\psi, n, p, Y_1, \ldots, Y_N), \quad J_{Y_i} = -\mu_i Y_i \nabla\psi - D_i \nabla Y_i$$

Electric potential

$$-\nabla(\varepsilon \nabla \psi(x)) = -q\left(p(x) - n(x) + N_D^+(x) - N_A^-(x)\right) - \sum_{i=1}^{N} q_i Y_i(x)$$

Recombination/ generation source terms

R_X **Include electron capture and hole capture by defect species and reactions between various defect species**

Electron emission/ capture

$Z^i \leftrightarrow Z^{i+1} + e^-$

Activation Energy

$$R_{[Z^i \to Z^{i+1}+e^-]} \propto \sigma_{[Z^i \to Z^{i+1}+e^-]} Z^i \exp\left(\frac{\Delta E_{[Z^i \to Z^{i+1}+e^-]}}{kT}\right)$$

Cross section

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